

January 25, 2007

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1617 Cole Boulevard  
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Re: NREL Subcontract #ADJ-1-30630-12  
D.5.8

Dear Bolko,

This report covers research conducted at the Institute of Energy Conversion (IEC) for the period of 9/16/06 to 10/16/06 under the subject subcontract. The report highlights progress and results obtained under Task 3 (Si-based Solar Cells).

### **TASK 3. SI-BASED SOLAR CELLS**

One of the key aspects of high efficiency silicon heterojunction (SHJ) solar cells (>21%) is the reduction of surface recombination by minimizing structural and electronic defects at the interface between amorphous silicon (a-Si:H) and crystalline silicon (c-Si) [1]. The deposition of very thin (< 10 nm) a-Si:H films in radio frequency (RF) plasma enhanced chemical vapor deposition (PECVD) or hot wire (HW) CVD on clean hydrogen terminated single crystalline Si wafers often starts with an unintentional growth of epitaxial layer, even without any hydrogen dilution at substrate temperature of < 200°C, which results in poor cell performances with low  $V_{OC}$  [2,3]. Epitaxial growth and defect passivation may depend on wafer orientation. It is therefore imperative to study the structure of the deposited Si:H layer and to correlate it with the passivation quality of Si surface with different orientations. In this work, we studied the surface passivation quality of a-Si:H intrinsic (i-) layers deposited with varying hydrogen dilution in RF and direct current (DC) PECVD process on float zone (FZ) n-type single crystalline Si (100) and (111) wafers.



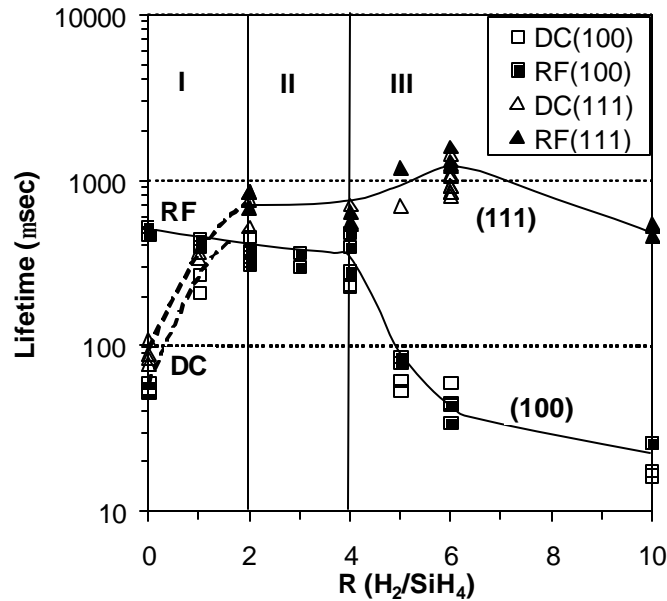
The Si wafers with resistivity of 1.0  $\Omega\cdot\text{cm}$  for (100) and 2.5  $\Omega\cdot\text{cm}$  for (111) were cleaned for 5 mins in a mixture of  $\text{H}_2\text{SO}_4\text{:H}_2\text{O}_2$  (4:1) followed by 5 mins rinse in de-ionized water and then in 10% HF for 30 sec prior to each Si:H deposition. The Si:H i-layers (10 nm) were deposited on both sides by RF and DC PECVD process using our multichamber system. The substrate temperature, deposition pressure and  $\text{SiH}_4$  flow rate were fixed at 200°C, 1250 mTorr and 20 sccm respectively, while  $\text{H}_2$  flow rate was varied from 0 sccm to 200 sccm. The RF power of 30 W and a plasma current of 123 mA for DC plasma were maintained constant. The effect of hydrogen dilution flow ratio  $R=[\text{H}_2/\text{SiH}_4]$  was studied. The quality of surface passivation was determined by measuring effective minority carrier lifetime [4]. Brewster Angle Fourier Transformed Infrared Spectroscopy (FTIR) and variable angle spectroscopic ellipsometry (VASE) measurement characterized the structure of the deposited layers on Si (100) and (111) wafers.

Figure 1 shows the minority carrier lifetime as a function of  $R$  for i-layers deposited on (100) and (111) wafers by DC and RF PECVD. It is worth mentioning here that the DC PECVD process will have a significantly higher ion bombardment compared to RF PECVD in otherwise similar plasma parameters due to higher plasma potential. Three distinct regions can be identified in the variation of lifetime with  $R$  (Fig. 1). In region I ( $R < 2$ ), the lifetime shows plasma process dependence but no orientation dependence. Namely, the DC plasma deposited i-layer at  $R = 0$  shows a much lower lifetime ( $< 100$  msec) and poorer surface passivation quality compared to the RF plasma deposited i-layers irrespective of the surface orientation. We speculate that increased contribution of higher order silane and heavy ion bombardment in the DC process at low  $R$  results in poor film quality due to excessive ion damage to the clean Si surface, thereby reducing lifetime. Formation of higher order silane decreases with increasing  $R$  in the DC plasma [5]. Also, higher  $R$  is expected to reduce ion bombardment due to increasing amount of lighter ions (ionic hydrogen instead of ionic Si containing molecules). Hence, the lifetime becomes similar for both RF and DC plasma deposited i-layers in region II and III ( $R > 2$ ). In region III ( $R > 4$ ), the measured lifetime exhibits a pronounced Si surface orientation dependence. For both RF and DC plasma, carrier lifetime sharply drops to  $< 100$   $\mu\text{sec}$  on (100) wafers for i-layers deposited with  $R > 4$ , while the lifetime on (111) wafers increases to  $> 1000$   $\mu\text{sec}$  for i-layers grown at  $R = 6$ . In order to get more insight about the variation of surface passivation quality with  $R$ , we have performed structural characterization of the deposited thin i-layers on Si (100) and Si (111) wafers.

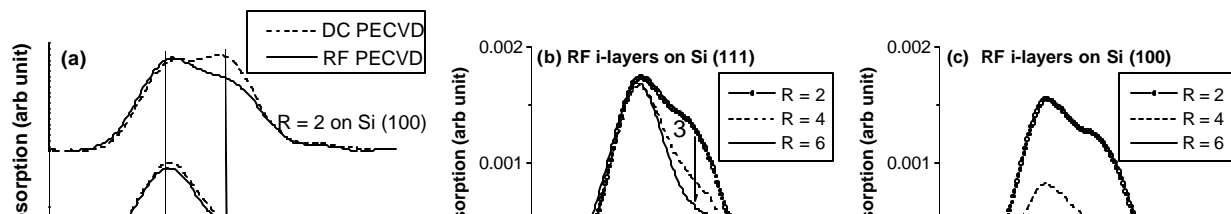
Figure 2(a) compares the FTIR spectra for RF and DC plasma deposited a-Si:H i-layers (10 nm) with  $R = 6$  on Si (111) and  $R = 2$  on Si (100) wafers. The peak intensities at 2090  $\text{cm}^{-1}$  and 2000  $\text{cm}^{-1}$  due to  $\text{SiH}_2$  and  $\text{SiH}$  stretching vibration respectively in i-layers deposited with  $R = 6$  are identical for both RF and DC plasma processes, which agrees well with the process independencies of carrier lifetime observed in Figure 1. The i-layer deposited with  $R = 2$  on Si (100) by DC plasma shows higher  $\text{SiH}_2$  bonding compared to RF plasma, indicative of poorer film quality presumably due to increased contribution from higher order silane in growth process. Figure 2 (b) shows the effect of  $R$  in FTIR spectra for i-layers deposited on Si (111) wafers by RF plasma. The figure exhibits an expected decrease of 2090  $\text{cm}^{-1}$  peak intensities with increase of  $R$ , which consequently increases carrier lifetime as shown in Figure 1. Figure 2 (c) shows hydrogen bonding of i-layers deposited on Si (100) surface with different  $R$ . The FTIR signals decrease with increase of  $R$  and i-layer grown at  $R = 6$  exhibit a very small signal with no detectable peak at 2000  $\text{cm}^{-1}$ , implying a large drop in total hydrogen content. Such a drop in FTIR signal for Si-H bonds indicates the deposited i-layer is nanocrystalline or epitaxial, which leads to sudden drop in carrier lifetime on Si (100) surface with i-layers deposited at  $R > 4$  (Fig.1).



Film thickness and structure of the deposited i-layers on Si (100) surface was also characterized by VASE measurement. Estimated thickness of amorphous phase of the i-layers deposited with  $R = 2, 4$  and  $6$  were  $10.8, 8.4$  and  $0$  nm respectively from VASE analysis; although the deposited film thickness measured on companion glass samples were  $10$  nm in all three cases. The Si:H layer deposited with  $R = 6$  has the same optical constants as crystalline silicon, which makes thickness estimation impossible from VASE. Figure 3 shows the variation of imaginary part of pseudo-dielectric function,  $\epsilon_2$  as function of photon energy for above three i-layers, assuming layer thickness of  $10$  nm. A broad featureless spectra for  $R = 2$  i-layer indicates the film is completely amorphous and i-layer grown at  $R = 4$  exhibits narrower peak with shift towards lower energy, indicative of mixed phase materials. Apparently thinner film estimated from VASE for  $R = 4$  i-layer can be due to an epitaxial growth at the initial stage of the deposition. The  $\epsilon_2$  spectra for  $R = 6$  i-layer is essentially identical to the crystalline silicon and suggests that the deposited layer is fully epitaxial. Therefore, a sharp decrease of carrier lifetime observed in Figure 1 for i-layers deposited at  $R > 4$  on Si (100) surface is due to epitaxial growth, which has a very poor passivation quality.

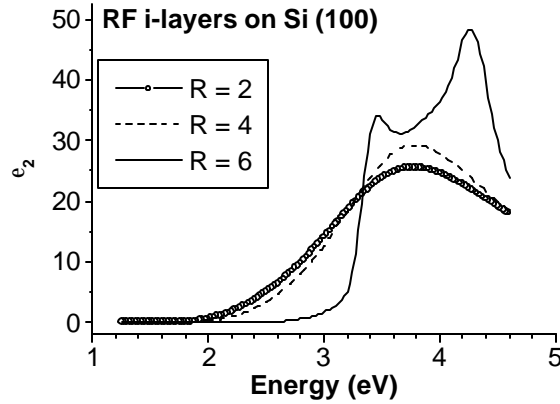


**Figure 1: Minority carrier lifetime on Si (100) and (111) wafers after depositing  $10$  nm Si:H i-layer on both sides by RF and DC plasma process with varying hydrogen dilution ( $R$ ).**





**Figure 2: Comparison of FTIR spectra for 10 nm Si:H i-layers; (a) films grown by RF and DC process; (b) RF layers on Si(111) wafer at different R; (c) RF layers on Si(100) wafer at different R.**



**Figure 3: Imaginary part of pseudo-dielectric function,  $\epsilon_2$  as function of photon energy for the Si:H layer deposited on Si(100) wafer at different R in RF plasma process.**

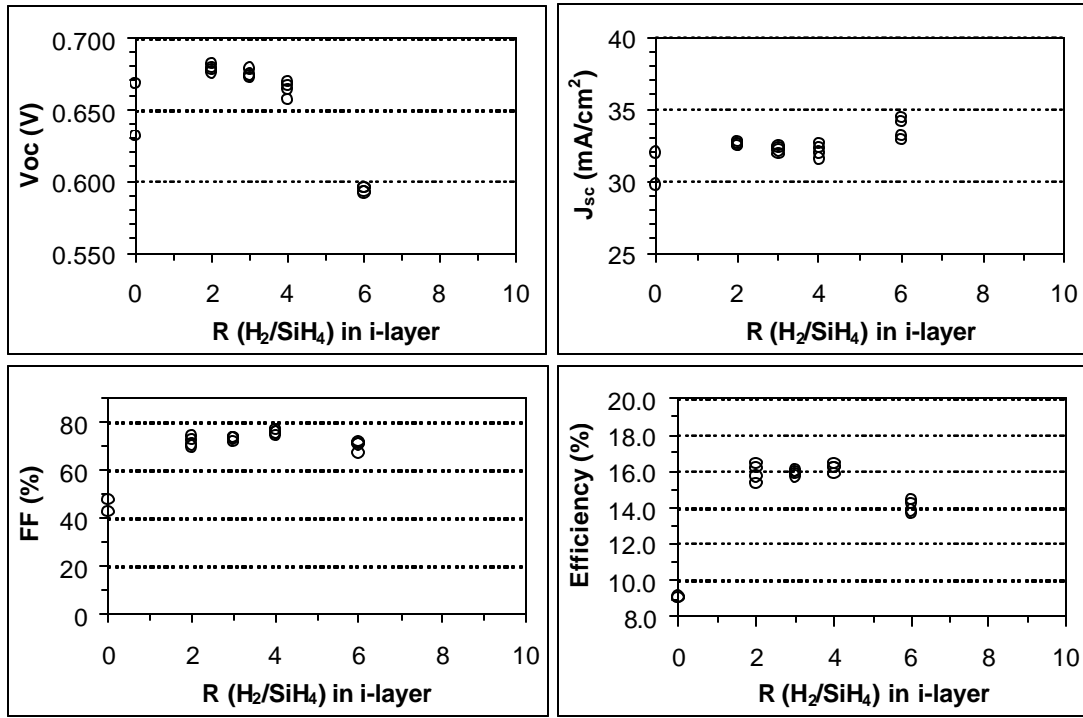
Solar cells were fabricated with 10 nm i-layers deposited on both sides by RF PECVD at different hydrogen dilution on n-type Si (100) wafers. The doped (p-type emitter and n-type BSF layer) a-Si layers were identical in all devices. Cells were completed with Al back contact and ITO with grids for the front contact. Device performance as a function of R is shown in Figure 4.

Low efficiency (<10%) shown for the cell with R = 0 i-layer is primarily due to very low FF (<50%) with an “S” shaped J-V curve. FTIR data shown above indicated that SiH<sub>2</sub> bonding and hydrogen content increases with the decrease of R. Therefore, at R = 0, the deposited layer is expected to have a wider band gap due to higher hydrogen content and presumably more defects due to more SiH<sub>2</sub> bonding. Observed non-ideal J-V characteristics can thus be due to highly defective i-layer and/or increased band gap, which enhances valence band offset at the hetero interface.



We achieved cell efficiency  $> 16\%$  for the i-layers grown with  $2 = R = 4$ , with highest  $V_{OC}$  of 682 mV for  $R = 2$ . The efficiency decreases to  $\sim 14\%$  for the cell with  $R = 6$  i-layer due to the drop in  $V_{OC}$  ( $< 600$  mV). Such drop in  $V_{OC}$  can be attributed to loss in surface passivation quality (minority carrier lifetime of  $< 100$  msec) of i-layer due to epitaxial growth on Si (100) surface at  $R = 6$ , as shown in Figure 3.

In conclusion, excellent surface passivation and high lifetime ( $> 1$  msec) can be achieved by both RF and DC plasma process with hydrogen dilution. Any epitaxial growth of the i-layer reduces minority carrier lifetime dramatically. The structure of thin Si:H layer depend on the orientation of single crystalline Si. Undesirable epitaxial growth of Si:H films is more likely to occur on Si (100) compared to (111) surface. The lower  $V_{OC}$  in SHJ cells for i-layers having epitaxial or mixed phase growth observed in literature is due to loss in surface passivation quality by Si:H layers [2,3].



**Figure 4: Silicon heterojunction (SHJ) solar cell parameters ( $V_{OC}$ ,  $J_{SC}$ , FF, and efficiency) as a function of  $R$  ( $H_2/SiH_4$ ) in i-layer deposited by RF PECVD on n-type c-Si (100) wafer. The doped layers (p-type emitter and n-type BSF) were deposited by DC PECVD and were the same for all cells.**

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Best regards,

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